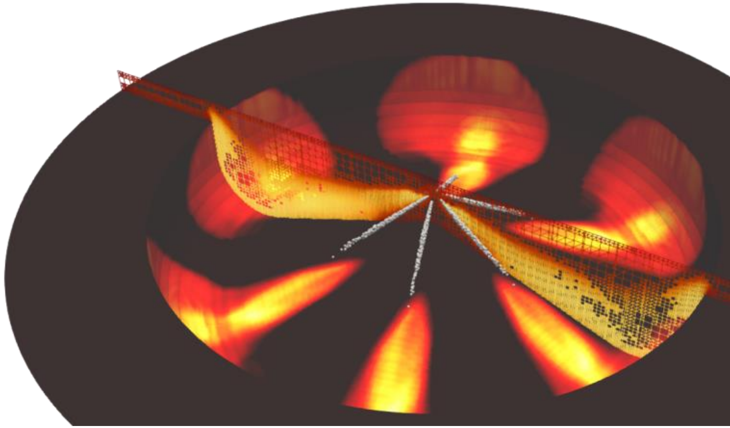
Towards Predictive Nozzle Flow and Combustion Simulations for Compression Ignition Engines



Gina M. Magnotti

P. Kundu, A.C. Nunno, S. Som (PI)

Argonne National Laboratory

Argonne Partners, Supported by Co-Optima

R. Torelli, H. Guo, C. Xu

Team Leader: Gurpreet Singh
Michael Weismiller
Kevin Stork

June 4th, 2020

Project ID # ACE135

Project Overview

Timeline

Project start: FY 2012
Part of 2017 VTO Lab Call

Budget

FY 16: $ 525 K
FY 17: $ 490 K
FY 18: $ 425 K *Funds reflect a reduced spending rate
FY 19: $ 300 K **Reduced budget reflects shift in project focus to heavy-duty applications
FY 20: $ 300 K

Barriers

- “Poor understanding of fuel spray fundamentals and accurate fuel spray submodels”
- “Inadequate simulation tools for accurately and robustly simulating advanced LTC*** processes”
- “Robust and accurate soot models are lacking”

Partners

Argonne National Laboratory
- Engines and Emissions Group
- Leadership Computing Facility (ALCF)
- Advanced Photon Source (APS)

Lawrence Livermore National Laboratory (LLNL)
Sandia National Laboratories (Sandia)
Convergent Science Inc. (CSI)
Cummins Inc.
Advanced Combustion and Emission Control (ACEC) **Technical Team**
Universitat Politècnica de València (CMT)

***LTC: Low Temperature Combustion

Relevance: Industry has voiced need for end-to-end simulation tool that can link fuel injector and engine performance with efficiency and emissions

Accuracy[1]	**Speed**[1]	**Availability**[1]
Flow internal to injector Cavitation-induced erosion Spray and mixing processes Autoignition and combustion Heat transfer Emissions (soot, NOx, etc.)	Reliable design tools with fast turn around times CFD* frameworks that can capitalize on HPC** resources	Design tools that can be seamlessly integrated into existing work flows

Objective: To address industry's needs, we develop simulation tools by leveraging experimental data from partners, ML*** tools, and HPC resources

Develop physics-based models:

Cavitation-Induced Erosion Risk Assessment Model (**CIERA**)[2]

Tabulated Flamelet Approach: Unsteady Flamelet Progress Variable (**UFPV**)

Identify bottlenecks and improve scalability of solvers and CFD codes:

Artificial Neural Network (ANN)-based acceleration toolbox[3]

Models published in open-literature, available to industry through software packages

Documentation of "engineering best practices" for using models and tools

[1] DOE-VTO workshop to identify roadmap for CFD organized by Leo Breton in 2014
[2] Magnotti, Som et al., ILASS-Europe, 2019
[3] Owoyele, Kundu et al., PROCI 2020
*CFD: Computational Fluid Dynamics; **HPC: High Performance Computing; ***ML: Machine Learning

Milestones and Project Updates for FY 20

Milestones

Date	Model	Milestone Description	Status
March 2020	Cavitation Erosion	Simulate cavitation and erosion in injector for comparison with X-ray experiments	**100% Complete**
September 2020	Combustion	Extension and validation of RIF-ist* code for split injections in constant volume experiments	**90% Complete**

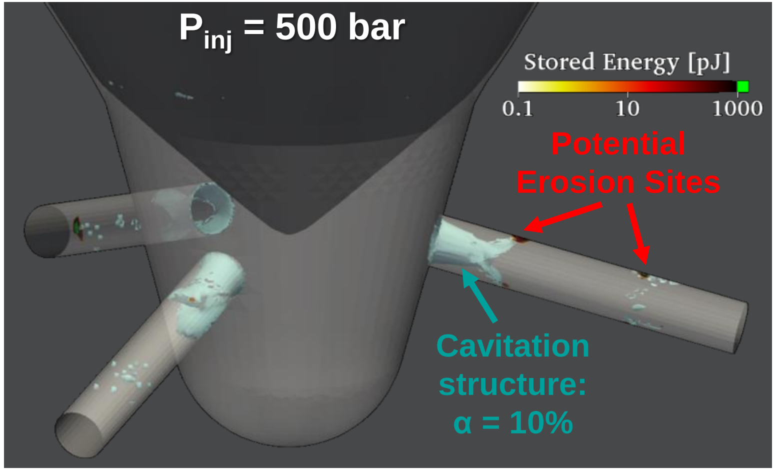
Project Updates

- Historically, this project has included a CRADA with Cummins and CSI. The CRADA expired at the end of FY19.
- We are in the process of renewing this CRADA for FY21 with Cummins and CSI, and adding Sandia (Dr. Lyle Pickett) and Argonne (Dr. Christopher Powell) as partners.

*RIF-ist: Representative Interactive Flamelet in-situ tabulation

Approach: Perform simulations of a multi-hole injector to study erosion and compare with X-ray images of endurance testing

Large Eddy Simulation (LES) of Nominal A-M3 Injector

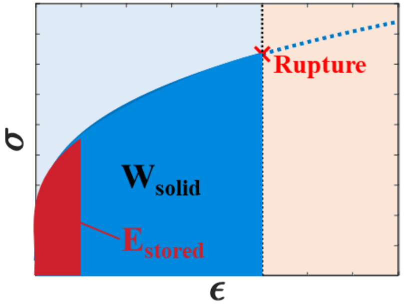


- Single-fluid mixture modeling approach with homogeneous relaxation model within CONVERGE used to capture cavitation development
- CIERA model[1,2] couples with multiphase flow predictions to predict critical erosion sites and erosion severity

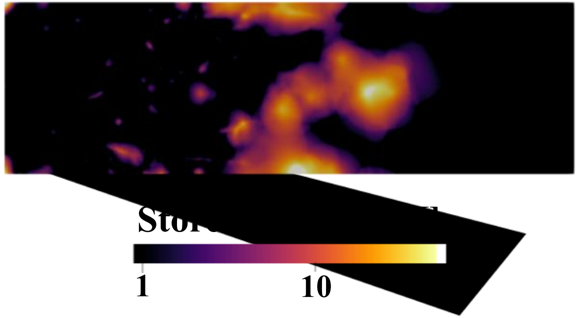
Cavitation-Induced Erosion Risk Assessment (CIERA) Model

Stress-Strain Curve

Solid material properties



After $t = \tau_{sim}$, evaluate E_{stored}



$$T \propto \frac{W_{solid}}{E_{stored}} \tau_{sim}$$

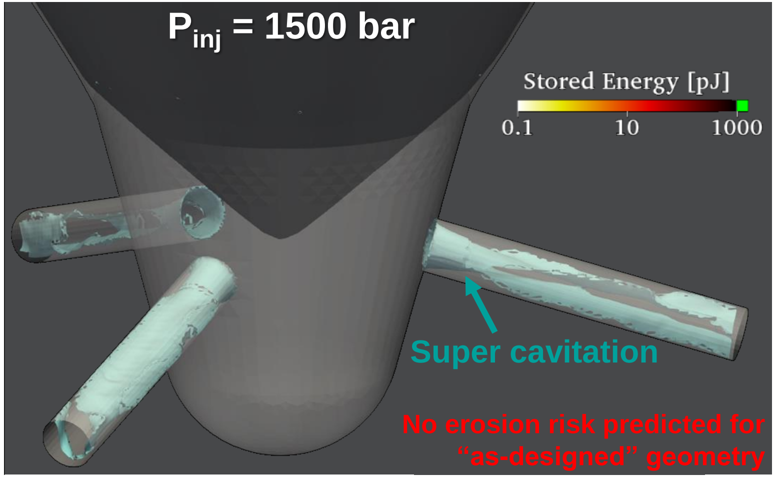
- In these exploratory studies, CIERA is employed as a *qualitative* metric to identify potential erosion locations
  - Yield strength is set to simulated injection pressure
- Studies are on-going to relate stored energy predictions to the solid material properties to *quantify* time to erosion

[1] Magnotti, Som et al., ICLASS, 2018
[2] Magnotti, Som et al., ILASS-Europe, 2019

Argonne NATIONAL LABORATORY

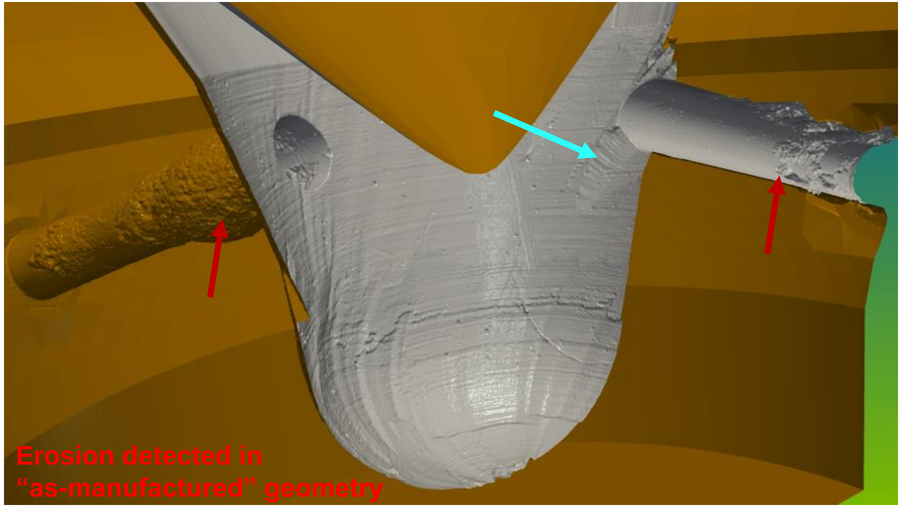
Accomplishment: Comparison of measured and predicted cavitation erosion highlight impact injector geometry and surface finish

Large eddy simulation (LES) of Nominal A-M3 Injector



- Using nominal geometry, prediction of super cavitation suppresses cavitation shedding and erosion
- X-ray scanned injector revealed large differences between "as-designed" and "as-fabricated" geometries
- Previous simulations[1] have shown sensitivity of cavitation and erosion to geometry and surface finish

X-ray Tomography of Eroded Aluminum Injector Tip[2]

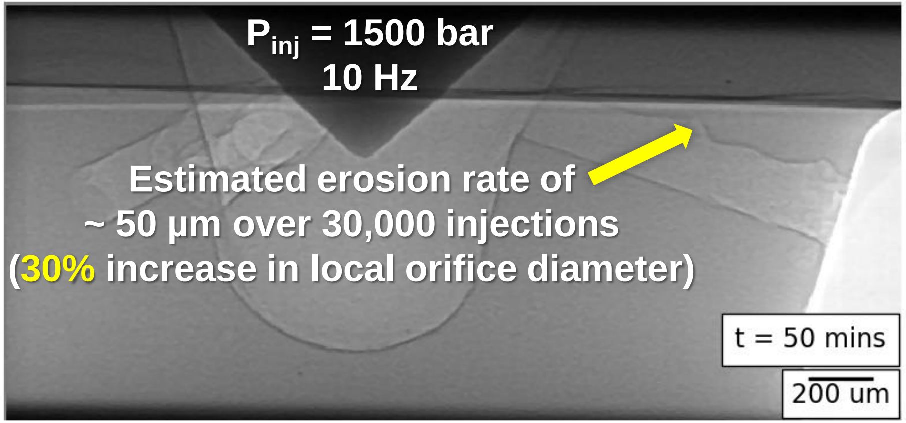


- Reconstructed geometry highlights details from **machining process** and level of **erosion** in orifices
- 3D surface used to inform computational domain and mesh for internal flow simulations

[1] Magnotti, Som et al., ICLASS 2018
[2] X-ray experimental data courtesy of Tekawade, Sforzo, Powell (Argonne)

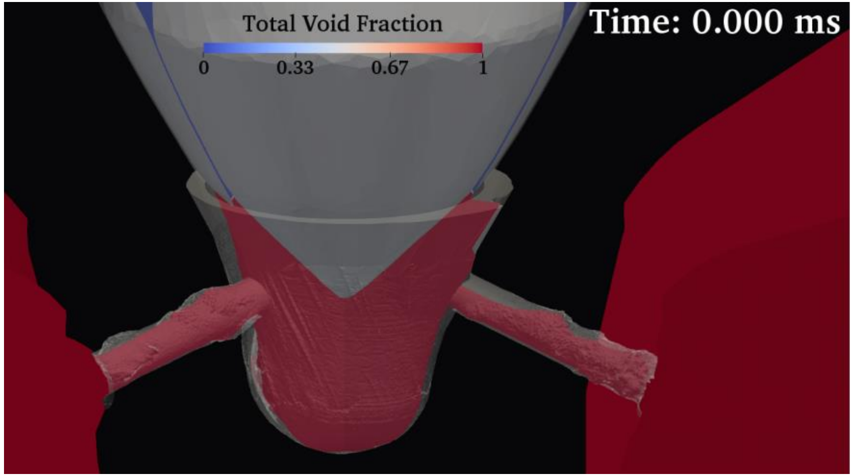
Accomplishment: First-of-its-kind simulations using an X-ray scanned eroded injector highlight impact of erosion on flow development

Synchrotron X-ray Imaging of A-M3 Injector Endurance Test[1]



- Injector tip fabricated from aluminum (A6060-T6)
- Erosion detected after 15 operating minutes (9000 injections)
- Preferential erosion on upper surface of orifice is observed for the hole of interest (but is not seen in the other orifices)

Simulations of Eroded AM-3 Injector



- Simulations indicate prolonged presence of cavitation formation, relative to simulations with nominal geometry
- Large differences in cavitation and erosion among orifices are likely due to geometric features from machining process
- Simulations are underway to understand impact of erosion on spray and combustion development

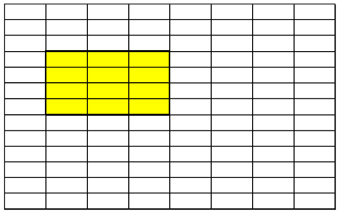
The use of X-ray informed geometries with multiphase flow simulation tools enables improved understanding of the relationship between erosion and injector performance

[1] X-ray experimental data courtesy of Tekawade, Sforzo, Powell (Argonne)

Approach: Model combustion with turbulence-chemistry interactions and full chemistry, at a fraction of the cost of WSR-MZ* model

Approach 1:

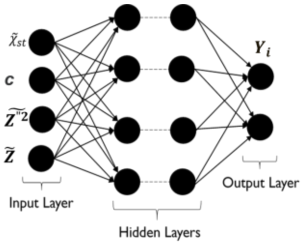
RIF-ist: Hybrid In-situ tabulation[1,2]



- A small part of the table is required at any given time-step
- Solve unsteady equations and re-generate table at each time-step based on local conditions

Approach 2:

UFPV: *A priori* tabulation with ANNs[3]



- Generate multi-dimensional flamelet libraries *a priori*
- **Significantly lower costs**
- UFPV approach recommended for industrial applications

ANL Flamelet Solver ⟷ Acceleration toolbox

ANL Flamelet Solver
- LSODES fast solver
- 2000+ species PAH** mechanisms
- Automated manifold regularizer
- Flamelet-coupled soot model
- 5D tables with unsteady flamelets

Acceleration toolbox
- Deep ANNs for accelerating flamelet models
- Autonomous manifold bifurcation using **Mixture of Experts**[4]
- **Significant memory reduction**

Flamelet Code

- **CONVERGE CFD**
  - RANS***/LES-based optimization
  - Internal nozzle coupled combustion modeling
  - ANN coupled flamelet framework in v3.0
- **Nek5000**

Argonne's flamelet solver + UFPV delivers the cost savings and accuracy required for industry's use of LES in engine simulations

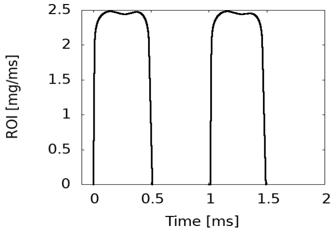
[1] Kundu et al. Comb. Sci. Tech 2019
[2] Ren, Kundu AIAA 2020-2089
[3] Owoyele, Kundu et al., IJER 2020
[4] Owoyele, Kundu et al., PROCI 2020

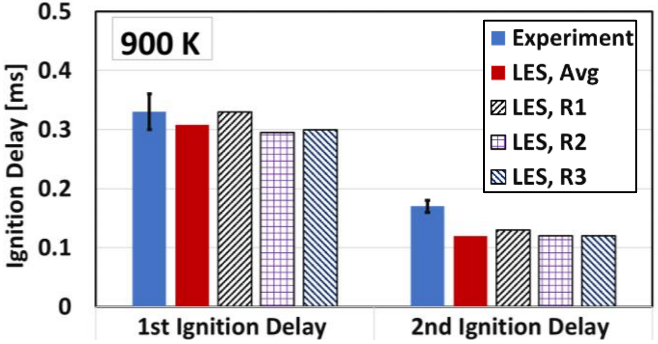
*WSR-MZ: Well-Stirred Reactor Multi-Zone; **PAH: Polycyclic Aromatic Hydrocarbons; ***RANS: Reynolds-Averaged Navier-Stokes

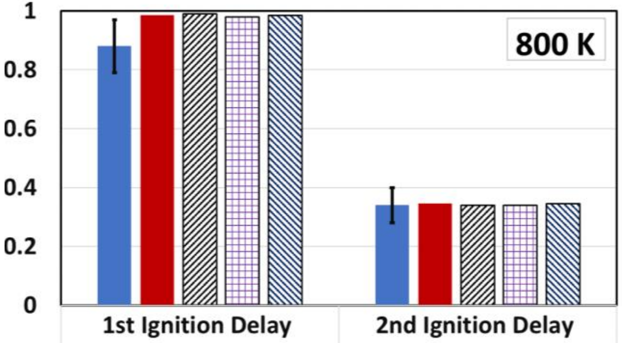
Accomplishment: Validation of UFPV code for multiple injections

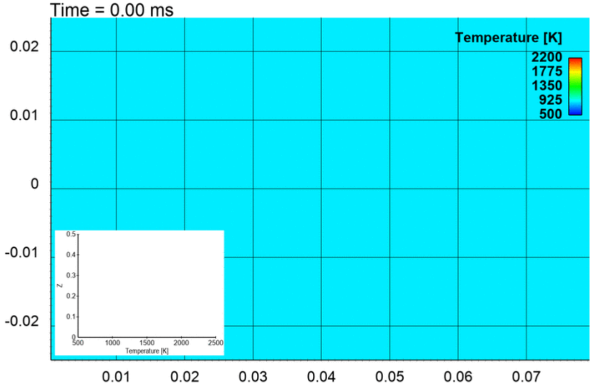
- **Extensive validation of in-house UFPV code against experimental data from Sandia[1]**
  - Demonstrated split injection simulations with full n-dodecane chemistry
  - Accurate predictions in autoignition and unsteady heat release during interaction phase
  - **UFPV has 3X* speed up over WSR-MZ with RANS**

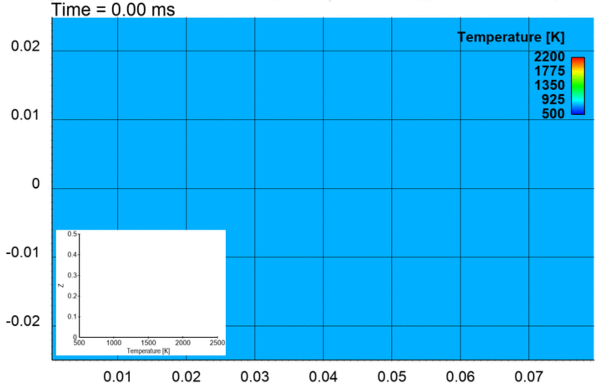
Parameter	Description
Fuel	n-dodecane
Chemistry mechanism (LLNL)[2]	**2,755 species**, 11,173 reactions
Tabulation	4D - $(\chi, c, \widetilde{Z''^2}, \tilde{Z})$
Finest Grid size	90 µm
Turbulence model	LES Dynamic Structure
Combustion model	UFPV
Ambient Temperature	750K, 800K, 900K
# realizations	3





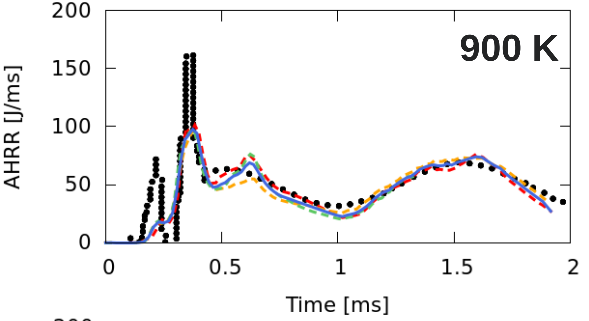






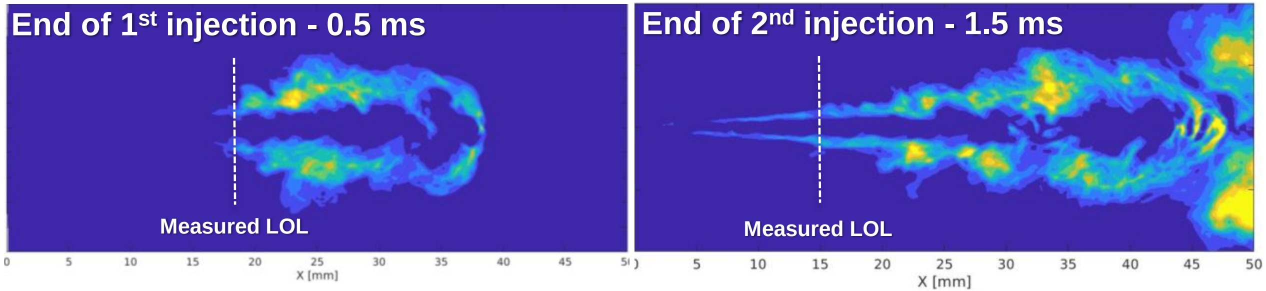
[1] Skeen et al., SAE Int. J. of Engines, 2015
[2] Sarathy et al., Combustion and Flame, 2011

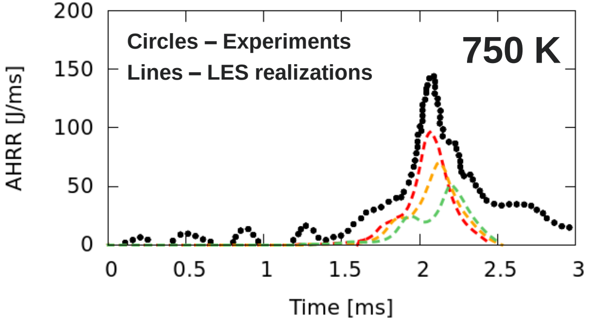
Accomplishment: Highly accurate predictions of heat release and combustion recession for multiple injections



- **Heat release rates (HRR):** Auto-ignition of the first jet characterized by a sharp spike in HRR, followed by a milder HRR for the second injection. The UFPV framework captures these interactions and TCI effects accurately.
- **Flame stabilization trends in split injection:** The liftoff lengths are predicted with high accuracy, along with the reduction in 2nd injection.

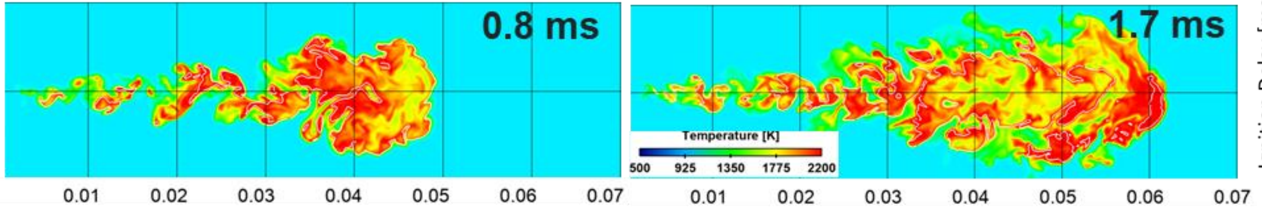
* Ensemble averaged OH mass fractions over **128 planes** and 3 LES realizations[1] (900 K)

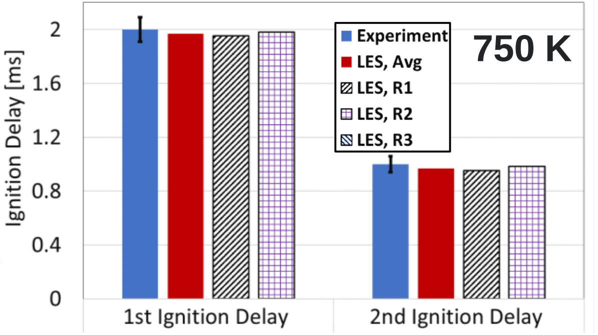




- **Combustion recession:** Recession observed after 1st and 2nd EOI captured accurately by the model

*Instantaneous temperature contours from LES realization (900 K)



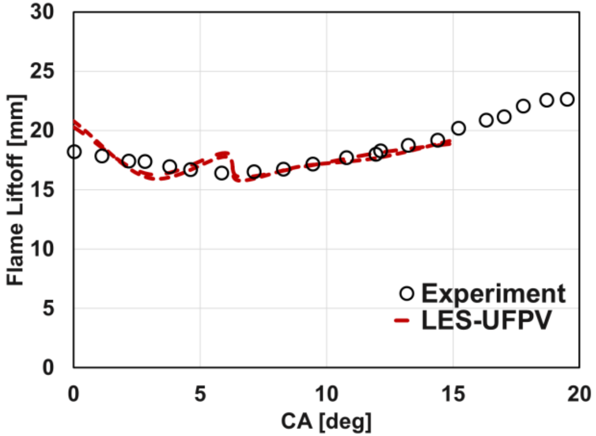


[1] Ameen, Pei, Som, SAE Technical Paper 2016-01-0585

Accomplishment: Demonstration of UFPV in Sandia's optical engine and integration of new soot modeling approach with UFPV in CONVERGE

Sandia optical-engine[1] simulations:

Parameter	Description
Fuel	Methyl-decanoate
Chemistry mechanism[2]	115 species, 460 reactions
Tabulation	5D - (P, χ, c, $\widetilde{Z''^2}$, $\tilde{Z}$)
Finest Grid size	90 µm
Turbulence model	Dynamic Structure LES



Interactive 2–way coupled flamelet-based soot model:

$$\rho \frac{\partial Y_i}{\partial t} + \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} = \dot{\omega}_i$$

$$\rho \frac{\partial T}{\partial t} + \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} = \dot{h}$$

$$\rho \frac{\partial Y_s}{\partial t} + \frac{1}{4}\left(\frac{\partial \rho \chi}{\partial Z} + \frac{\chi}{D_Z} \frac{\partial}{\partial Z}(\rho D_Z)\right)\frac{\partial Y_s}{\partial Z} = -\sqrt{\frac{\chi}{2 D_Z}} \frac{\partial}{\partial Z}(\rho Y_s V_s) + \dot{\omega}_{Y_s}$$

$$\rho \frac{\partial N_s}{\partial t} + \frac{1}{4}\left(\frac{\partial \rho \chi}{\partial Z} + \frac{\chi}{D_Z} \frac{\partial}{\partial Z}(\rho D_Z)\right)\frac{\partial N_s}{\partial Z} = -\sqrt{\frac{\chi}{2 D_Z}} \frac{\partial}{\partial Z}(\rho N_s V_s) + \dot{\omega}_{N_s}$$

- Store soot formation source terms in manifold
- **First implementation** of such an approach for soot calculations in engine simulations and commercial code
- Our solvers were used by collaborators at CMT-Valencia to demonstrate soot modeling capabilities[3]
- **3-10 X** speed-up for soot simulations over WSR-MZ

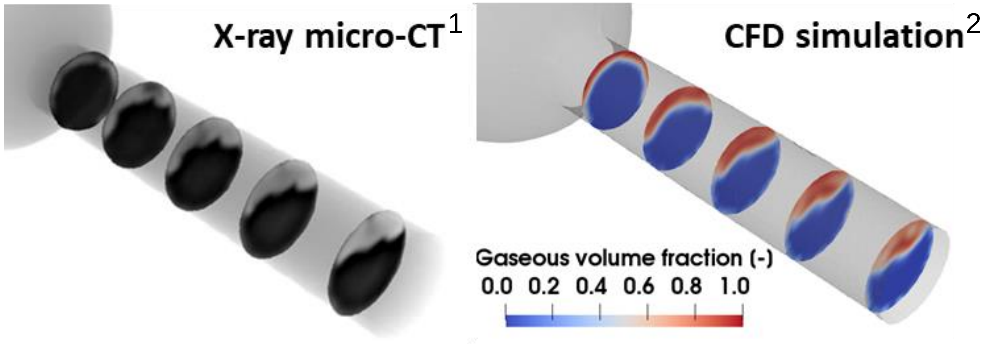
Framework helps in charting a path towards a robust and accurate soot modeling capability

[1] Cheng, Mueller et al., Energy & Fuels, 2014
[2] Luo, Som, Pitz et al., Fuel, 2012
[3] Pachano L., PhD Thesis, CMT-Valencia, 2020

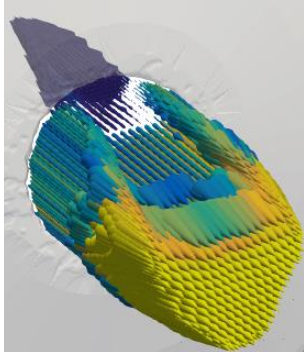
Approach: Develop best practices for using static coupling to link internal flow details with external spray development

- **High fidelity internal nozzle flow simulations of the ECN Spray C injector were performed under realistic conditions to generate detailed flow information at the nozzle exit**
- **Best practices under development for static coupling of nozzle flow and the ensuing spray**
  - X-ray measurements of injector geometry and 3-D transient needle motion used to provide accurate boundary conditions for nozzle flow simulations
  - Nozzle exit conditions (velocity, temperature, void fraction) predicted by internal flow simulations used to initialize the Lagrangian spray simulation
  - Large eddy simulations were performed for both internal flow and spray modeling with minimum grid sizes of 10 μm in orifice and 62.5 μm in outer chamber, respectively

Experimental and predicted gas layer distribution inside orifice



Flow information at nozzle exit



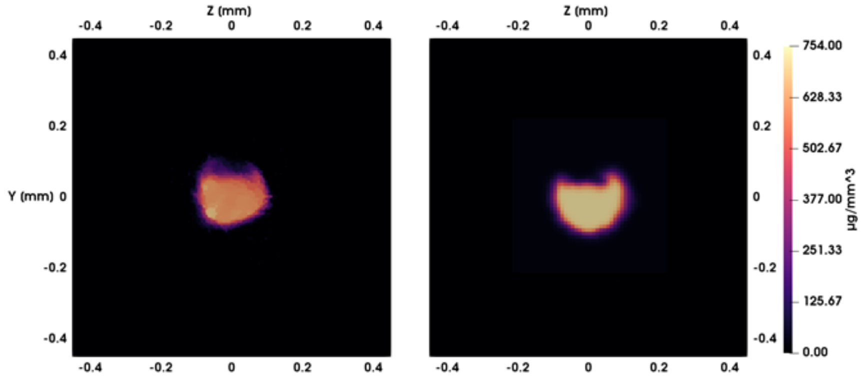
[1] Tekawade, Powell et al., Scientific Reports, Accepted
[2] Guo, Torelli et al., SAE Technical Paper 2020-01-1154

Accomplishment: Near-nozzle spray characteristics validated against X-ray data using static coupling approach

- **Validated near-nozzle liquid density profile against X-ray data**
  - Nozzle flow simulation provided accurate nozzle exit conditions to initialize spray modeling
  - Static coupling allows for internal flow structure to be propagated to mass distributions in external sprays, with peak density and spread in agreement with experiments
  - The link between internal flow structure and spray development cannot be captured using the standard rate-of-injection approach to define the injection velocity

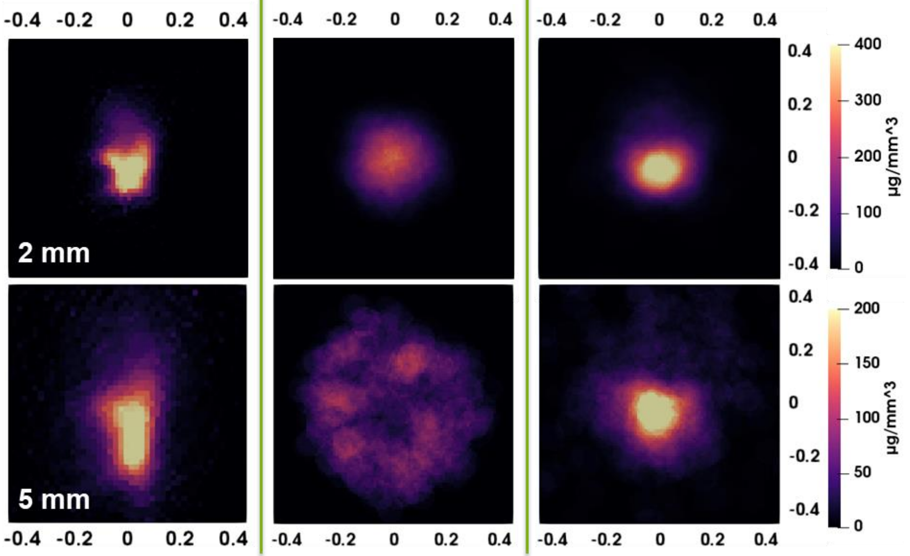
Liquid density profile at the nozzle exit

X-ray radiography[1] (ensemble averaged) | **Nozzle flow simulation** (single injection event)



Liquid density profile outside the nozzle

X-ray radiography | **Rate-of-injection** | **Static coupling**

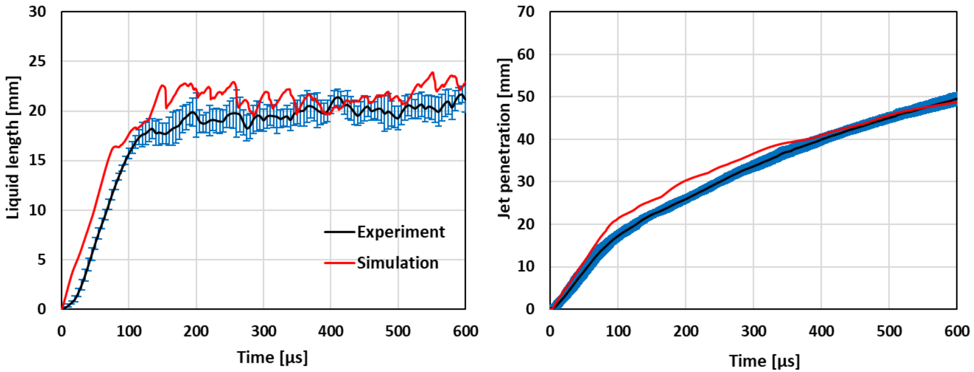


[1] Sforzo, Powell et al., ILASS-Europe, 2019

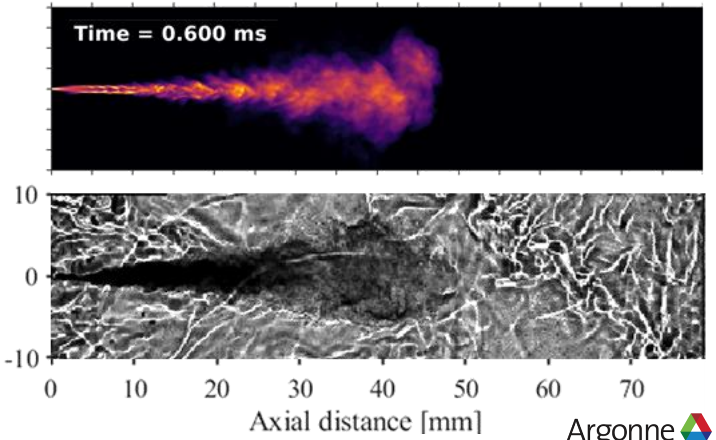
Accomplishment: Best practices under development for static coupling method via comparison with ECN Spray C data

- **The static coupling approach showed good prediction of liquid length and jet penetration during the late injection period under the Spray C non-reacting condition**
  - Minimum grid size of 62.5 μm used in the simulation to achieve grid convergence
  - Parcels initialized with specified turbulent kinetic energy to match the cone angle
  - On-going work is focused on modeling <u>injection transients</u> by simulating injector with lower initial needle lift (~2.5 μm) to better represent flow conditions in the sac and orifices and reduce initial fuel mass delivery
- **This work demonstrates static coupling approach for linking internal flow behavior with external spray development, with a path to improving best practices for use by industry**

Measured and predicted liquid and jet penetration



Spray images from CFD and experiment[1]



[1] Engine Combustion Network, https://ecn.sandia.gov/

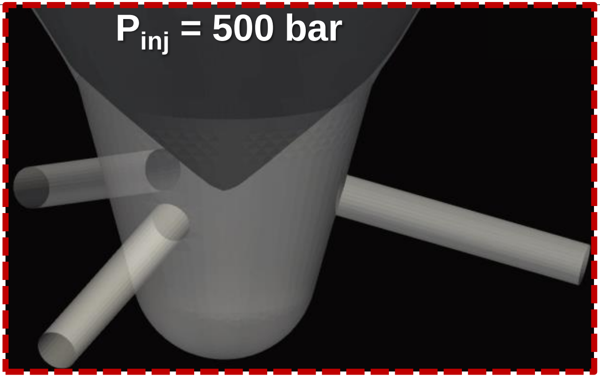
Accomplishment: Demonstration of end-to-end tool that couples in-nozzle flow with spray and combustion development

- **Framework developed to integrate latest advances in cavitation and turbulent combustion modeling**

Multiphase Flow Modeling
- Cavitation & CIERA
- X-ray scanned geometry
- Transient needle dynamics

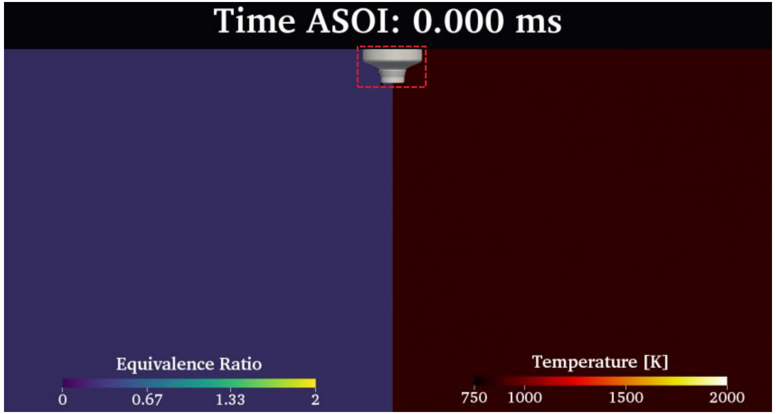
Combustion Modeling
- 2000+ species PAH mechanisms
- TCI* and LTC
- Detailed surrogates, soot models

Coupled Framework
Ability to link injector performance with resultant mixing field, combustion development, and pollutant formation



Injection Conditions

Void Fraction
Velocity
Injected Mass
Temperature



Demonstration of injection from nominal 3-hole injector, coupled with UFPV combustion model using a RANS turbulence model (1500 cpu-hrs)

- Developed simulation tool shows promise in linking injector and engine performance with efficiency and emissions, but further development is still needed to enable its routine use by industry
- Coupled simulation predictions should be validated against detailed spray and combustion experiments

*TCI: Turbulence-Chemistry Interaction

Response to Previous Year Reviewers' Comments

Overall, the reviewers were positive about the project:

"The PIs have identified problems of great significance through collaborations with experiments and interactions with industry, and their approach to modeling these issues…is quite good."

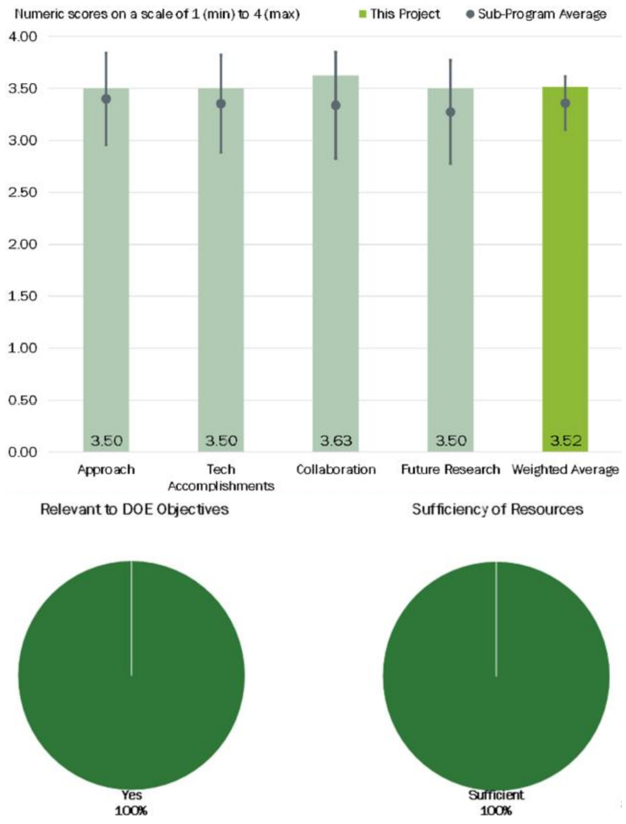
The reviewers noted suggestions for increasing the impact of project.

One reviewer suggested for the PIs to generalize hybrid tabulation flamelet framework to consider any number of injections, given complex injection schedules used in modern engines.

The coupling of Argonne's flamelet solver with UFPV has been generalized for multiple injections and demonstrated for simulating a double injection case in a spray vessel and in an engine.

One reviewer suggested for the PIs to continue with uncertainty quantification (UQ) for all aspects of the project to enhance collaboration with experiments.

Application of UQ to engine simulations remains a challenge due to the compounding effects of epistemic (model) and aleatoric (intrinsic randomness) uncertainty, and need for large datasets. We continue to leverage HPC resources and are exploring the use of ML tools to perform UQ in our simulations. To evaluate epistemic uncertainty, we plan to collaborate with Dr. Muhsin Ameen (Argonne) to leverage their Nek5000 spray and turbulence predictions and Dr. Jackie Chen (Sandia) to leverage their DNS flame predictions. Close collaborations with experimentalists will allow us to better characterize aleatoric uncertainty in boundary and initial conditions.



Collaboration and Coordination with Other Institutions

Argonne National Laboratory

- **Engine and Emissions Group: (Provide data for model validation)**
- **Leadership Computing Facility (Improving scalability of CONVERGE, HPC resources, ML and data science tools)**
- **Advanced Photon Source: (Nozzle flow and spray data, CRADA*)**

Lawrence Livermore National Laboratory (n-dodecane mechanism with PAH chemistry)

Sandia National Laboratories (Spray combustion and optical engine data, CRADA*)

Convergent Science Inc. (Algorithm and code development in CONVERGE, CRADA)

Aramco Research Center (Argonne erosion model leveraged for injector simulation studies)

Caterpillar Inc. (Argonne combustion tools led to collaboration in HPCEI project)

Cummins (Provide experimental data, alpha testing of new models, CRADA)

Navistar (SuperTruck program leverages modeling tools developed in this project)

CMT-Universitat Politècnica de València (Argonne flamelet solver leveraged for spray and soot simulations)

Georgia Institute of Technology (Accelerating internal flow simulations by developing ML-based emulator)

Presentations at Advanced Engine Combustion (AEC) Working group
Engine Combustion Network (ECN) participation and data contribution

***Simulation Toolkit Team* in "Co-Optima" and simulation teams in Partnership for Advance Combustion Engines (PACE) are leveraging our developments in multiphase flow and combustion modeling**

***Collaboration in CRADA to begin in FY21**

Remaining Challenges and Barriers

- Internal nozzle flow: Internal flow simulations of injectors are still a computational bottleneck in producing accurate injection conditions, such as those that are needed for the end-to-end simulation tool. Internally funded project at Argonne and collaboration with Georgia Tech (Prof. Vigor Yang) focus on developing ML-based emulators to expedite injector simulations.

- Cavitation erosion: Extremely disparate time scales between cavitation and material fatigue leading to erosion. Collaborating with material scientists may provide insight into observed erosion patterns and recommendations for representing evolution of stress-strain profile in material.

- High-fidelity injector and engine experimental data: We need dedicated experiments to validate some of our models and at times these data are not available and need to be generated. Also, we need uncertainties in measured data. Simulations do not account for the experimental uncertainties that can be significant at times.

- Uncertainty quantification (UQ): Rigorous UQ has not yet been applied to engine CFD simulations to understand compounding effects of epistemic (model) and aleatoric (intrinsic randomness) uncertainty. Provided sufficient data, machine learning tools show promise in addressing this need.

- Soot modeling: It is extremely challenging to capture soot formation in CFD simulations in a predictive fashion. It requires the accurate modeling of a large number of coupled processes, incorporation of detailed PAH chemistry and detailed soot models. Disparate chemical time scales associated with species and slow forming PAH species render traditional flamelet tabulation approaches to be inaccurate. Estimating particle size distribution is also a significant challenge.

Proposed future work* charts a path to further development of simulation tools for designing next-generation engines

Improving Modeling Tools for Fully Coupled Simulations (*CRADA - Argonne, Sandia, Cummins, and CSI*)

- 3 year project will focus on high-resolution injector flow LES and companion X-ray and optical experiments to enable predictive, *dynamically* coupled injector-spray combustion simulations using Eulerian Lagrangian Spray Atomization (ELSA) model
- Improve underlying atomization model and transition criteria in ELSA model, applicable to multi-hole injectors

Cavitation Erosion Modeling

- Validate CIERA predictions for steady state erosion rate in multi-hole injector against X-ray experimental data over a range of operating conditions and materials
- Investigate influence of eroded geometry on external spray and combustion characteristics
- Use validated injector model to propose and test design changes that reduce erosion severity

Turbulent Combustion Modeling

- Incorporate detailed soot modeling approaches (e.g. Method of Moments), while lowering costs, to expedite industry’s adoption of latest simulation tools. Validate predictions using engine data with multi-pulse injections.
- In collaboration with Dr. Jackie Chen (Sandia), use DNS data from split injection scenarios to assess flamelet model formulations and assumptions and inform improvements to the model. Use validated flamelet model predictions to provide more realistic boundary and operating conditions for future DNS studies.

***Any proposed future work is subject to change based on funding levels.**

Summary

Objective

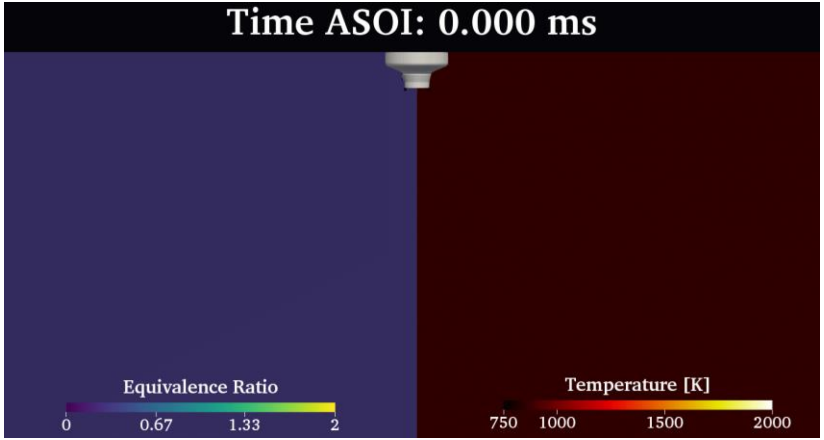
- Development of predictive, fully coupled spray, turbulence, and combustion models, informed by comprehensive validation and aided by HPC and ML tools

Approach

- Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC and ML resources for development of robust engine models

Collaborations and coordination

- With industry, academia, and national laboratories
- Through VERIFI, collaborations with light-duty, heavy-duty, software vendors, and energy companies



End-to-end simulation capability demonstrated for multi-hole injector using static coupling and UFPV

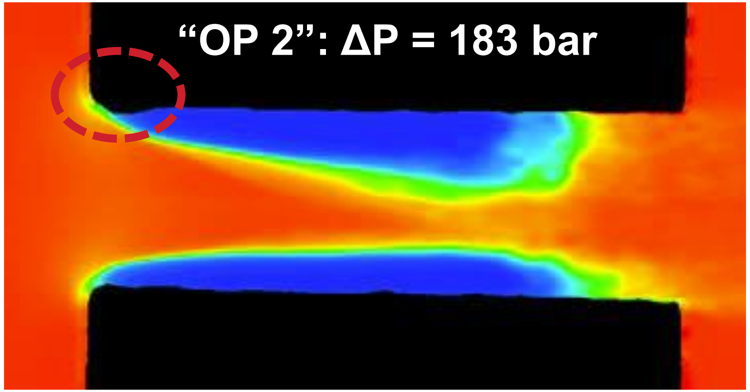
Technical Accomplishments

- Validated internal flow and near-nozzle spray predictions of the ECN Spray C injector against X-ray data informed development of best practices for coupling injector flow and spray predictions
- First-of-its-kind simulations of an X-ray scanned eroded injector highlighted the impact of erosion on internal flow development and fuel mass delivery
- Integration of Argonne’s flamelet solver with UFPV provided accurate predictions in spray and engine at a fraction of the cost of the industry-standard approach, thus outlining a path for routine use of LES in engine simulations
- UFPV was coupled with a 2-way soot model to enable detailed chemistry and soot predictions

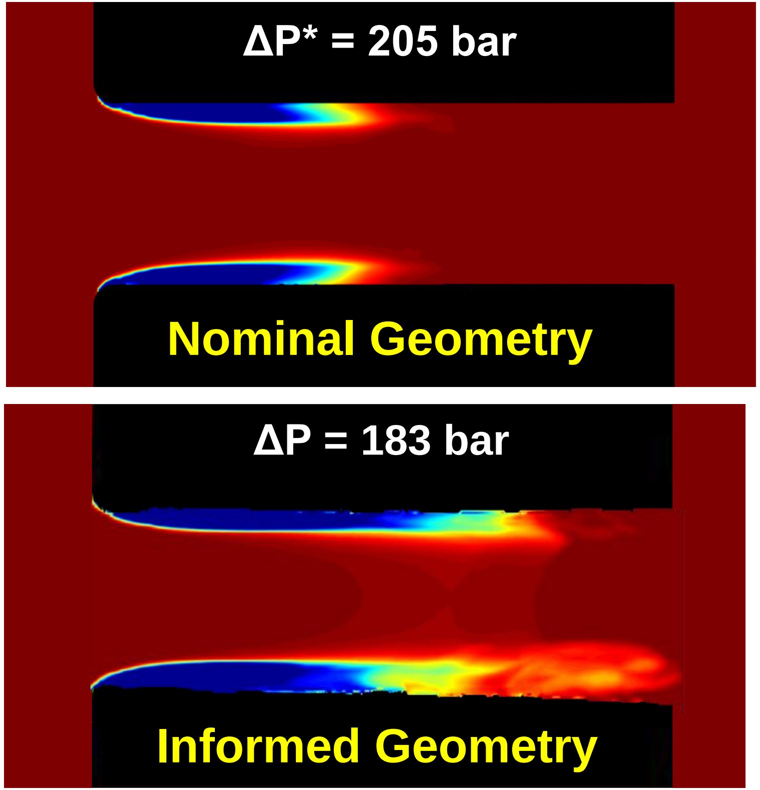
Technical Backup Slides

Accomplishment FY18: Simulations show importance of using realistic geometry in order to capture cavitation development

Experimental Observation



Simulation Predictions

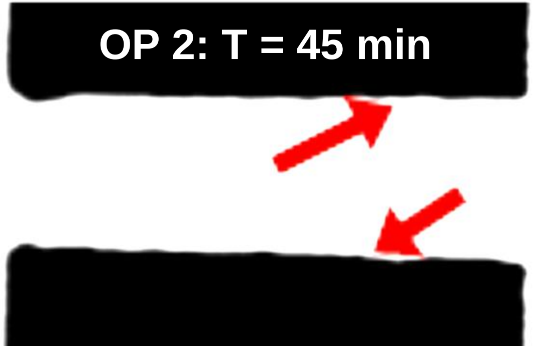


Using the geometry informed from the experimental images, good agreement was achieved with respect to cavitation development

[1] Skoda et al., WIMRC 3rd Int. Cavitation Forum, 2011.
[2] Magnotti, Som et al., ICLASS 2018.

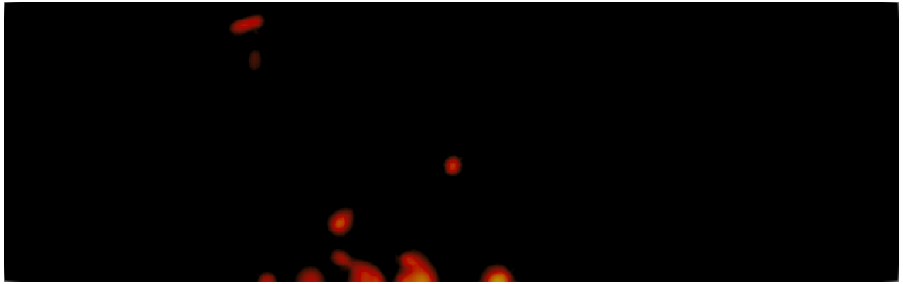
Accomplishment FY18: Higher erosive potential is predicted by informed geometry relative to the nominal geometry

Measured Cavitation Erosion[1]



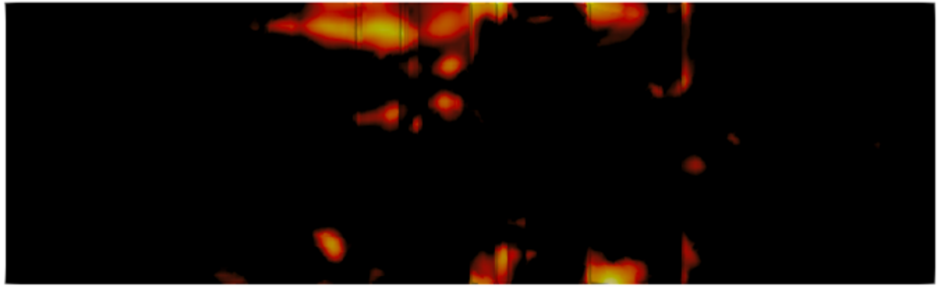
Nominal Geometry

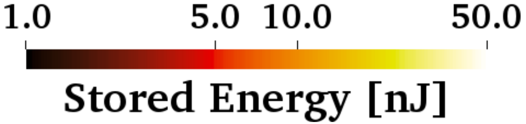
ΔP* = 205 bar



Informed Geometry

ΔP = 183 bar

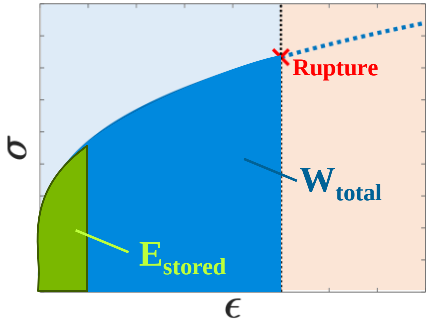




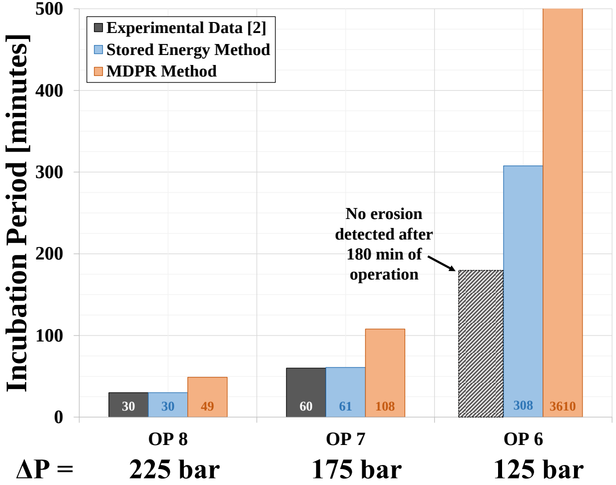
[1] Skoda et al., WIMRC 3rd Int. Cavitation F
[2] Magnotti, Som et al., ICLASS, 2018.

Accomplishment FY19: Erosion severity accurately predicted over several flow conditions

- In order to calculate an incubation period, T, cavitation erosion predictions must be related to solid material properties
- For a given material, the total work required for the solid to undergo rupture, W_{total}, can be calculated through integration of the stress-strain curve while accounting for strain-hardening effects
- The ratio of W_{total} to the predicted E_{stored} is used to scale the simulated time, $\tau_{simulated}$, and estimate T
- In the standard approach using the mean depth penetration rate (MDPR) method, the mean stress is used to characterize hydrodynamic impacts and estimate T
- Evaluation of the two methods across a range of ΔP conditions highlights the improved prediction capability with the newly developed stored energy method due to its dependence on both impact strength and duration
- Assumed level of non-condensable gas concentration has been noted to have a strong effect on the predicted incubation period and response to changes in flow conditions



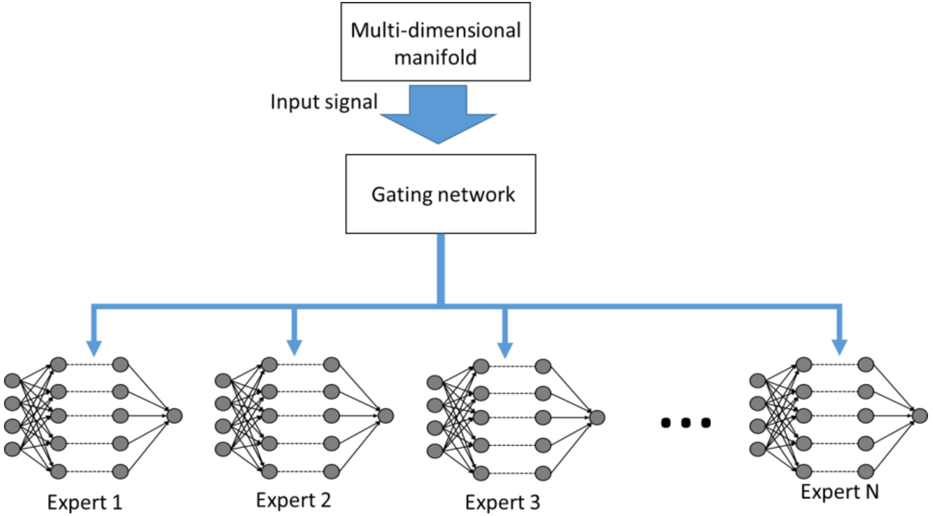
$$T \propto \frac{W_{total}}{E_{stored}} \tau_{simulated}$$

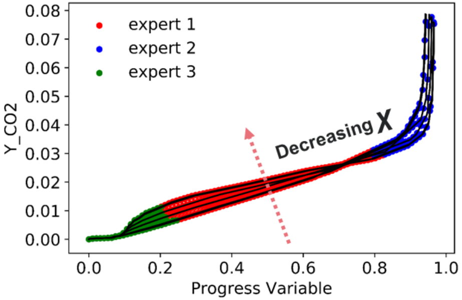


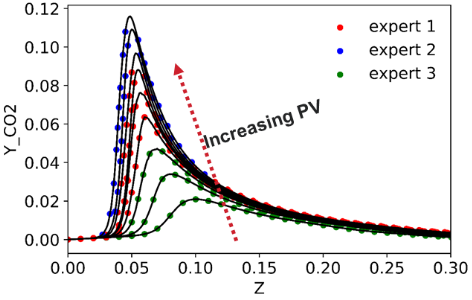
[1] Magnotti, Som et al., ILASS-Europe 2019
[2] Skoda et al., WIMRC, 2011

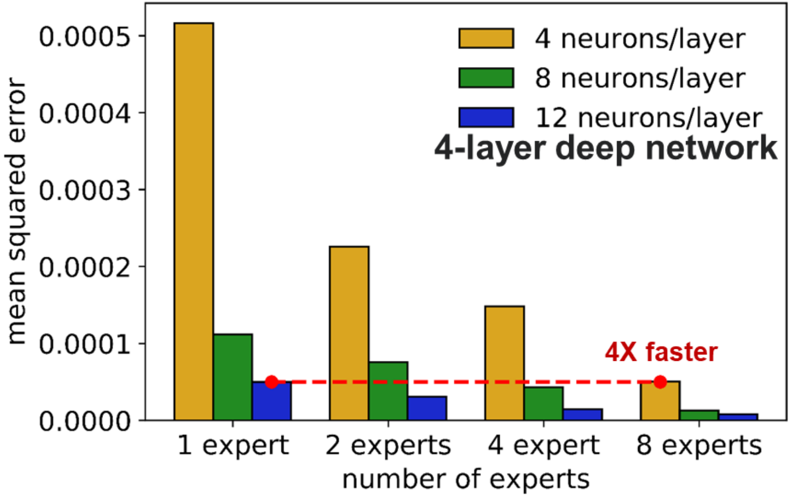
Mixture of Experts Framework[1]

Autonomous manifold bifurcation







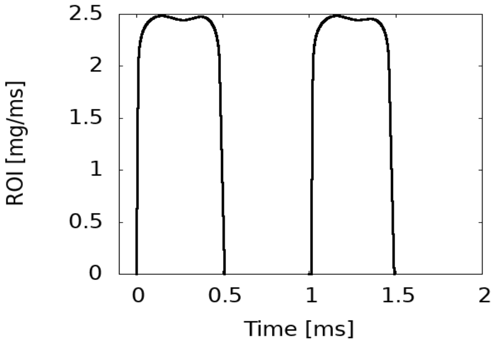


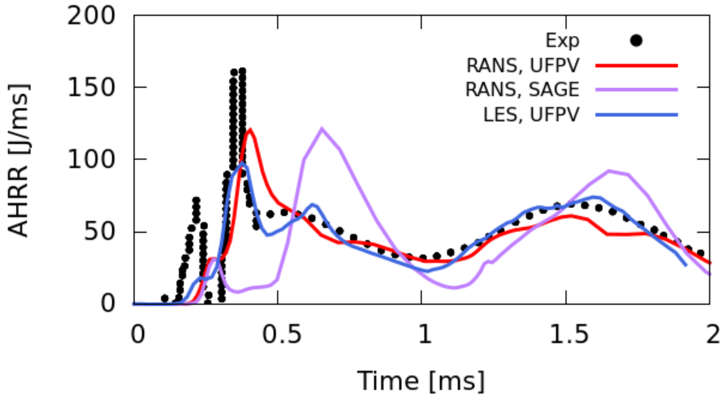
- Divide and conquer approach for automated bifurcation of N-dimensional manifold
- 4X faster inference than traditional formulation
- Can be automated for any type of problem, application or manifold
- Develop a standalone *"manifold compression tool"* that can be used by any code and application

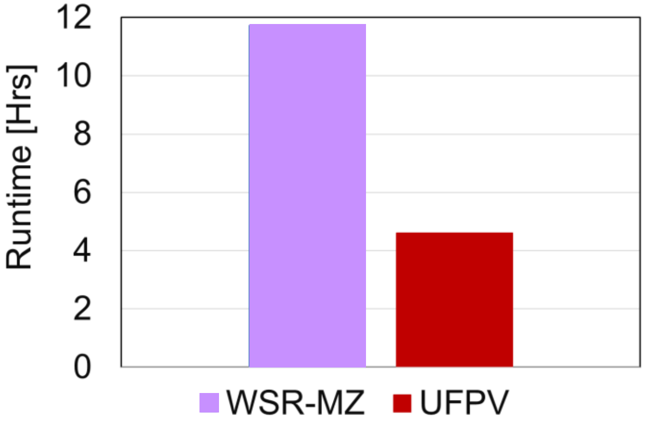
[1] Owoyele, O., Kundu, P., & Pal, P. Efficient bifurcation and parameterization of multi-dimensional combustion manifolds using deep mixture of experts: an a priori study. Proceeding of the Combustion Institute 2020. (accepted)

Comparison of computational cost and accuracy of combustion modeling approaches for double injection simulation

Parameter	Description
Fuel	n-dodecane
Chemistry mechanism [1]	**103 species, 370 reactions**
Combustion Model	WSR-MZ (SAGE) and UFPV
Finest Grid size	0.25 mm
Turbulence model	RNG k-epsilon
Ambient Temperature	900 K
Number of processors	32







[1] Luo et al., Comb. Theory and Modeling 2014.

Argonne NATIONAL LABORATORY